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Analysis and Computation of the Derivative Function for an Isolated Lorentz Line

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20 March 1979

Interim Report

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This report has been reviewed by the Information Office (OI) and is releasable to the National Technical Information Service (NTIS). At NTIS, it will be available to the general public, including foreign nations.

This technical report has been reviewed and is approved for publication. Publication of this report does not constitute Air Force approval of the report's findings or conclusions. It is published only for the exchange and stimulation of ideas.

Gerhard E. Aichinger
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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Analysis and methods of computation of the function

$$y(x,\rho) = \frac{2}{\pi}\int_0^{\infty} \exp\left(\frac{-2x}{1+\rho^2 z^2}\right)\frac{dz}{1+z^2}$$

rho

are presented. Power series, asymptotic series, and other expansions are developed for six regions of the positive quadrant of the xρ plane. These expansions allow efficient calculation of y(x,ρ) to a relative accuracy of 0.01% or better.

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CONTENTS

INTRODUCTION

Treatment of radiative transfer for an isolated Lorentz line in the Lindquist-Simmons approximation[1,2] requires the evaluation of the derivative function $y(x, \rho)$ defined by

$$y(x, \rho) = \frac{2}{\pi} \int_0^\infty \exp\left\{-\frac{2x}{1 + \rho^2 z^2}\right\} \frac{dz}{1 + z^2} \tag{1a}$$

or, with the change of variable $\tan(\theta/2) = \rho z$, by

$$y(x, \rho) = \frac{2\rho}{\pi} \int_0^\pi \frac{e^{-x(1+\cos\theta)}}{(\rho^2 + 1) + (\rho^2 - 1)\cos\theta} d\theta . \tag{1b}$$

This same function is used in the resonance absorption band model formulation of Cobb.[3] In both applications, x is a measure of optical depth, and ρ is a ratio of line widths. The range of both x and ρ is zero to infinity.

Prior work on the evaluation of $y(x, \rho)$ includes the rational approximation of Lindquist and Simmons[1] (accuracy not stated), the tabulation of Young[2] (accuracy of one part in 10^5), and the series expansions of Cobb[3] (accuracy of < 1% for $0.01 \le x \le 10^5$, $10^{-3} \le \rho \le 10^3$, and $10^{-3} \le y \le 1$). The present work considers the efficient calculation of $y(x, \rho)$ to a relative accuracy of $\le 0.01\%$ for the entire positive quandrant of the $x\rho$ plane.

The general features of the function are shown in Fig. 1. The function limits are

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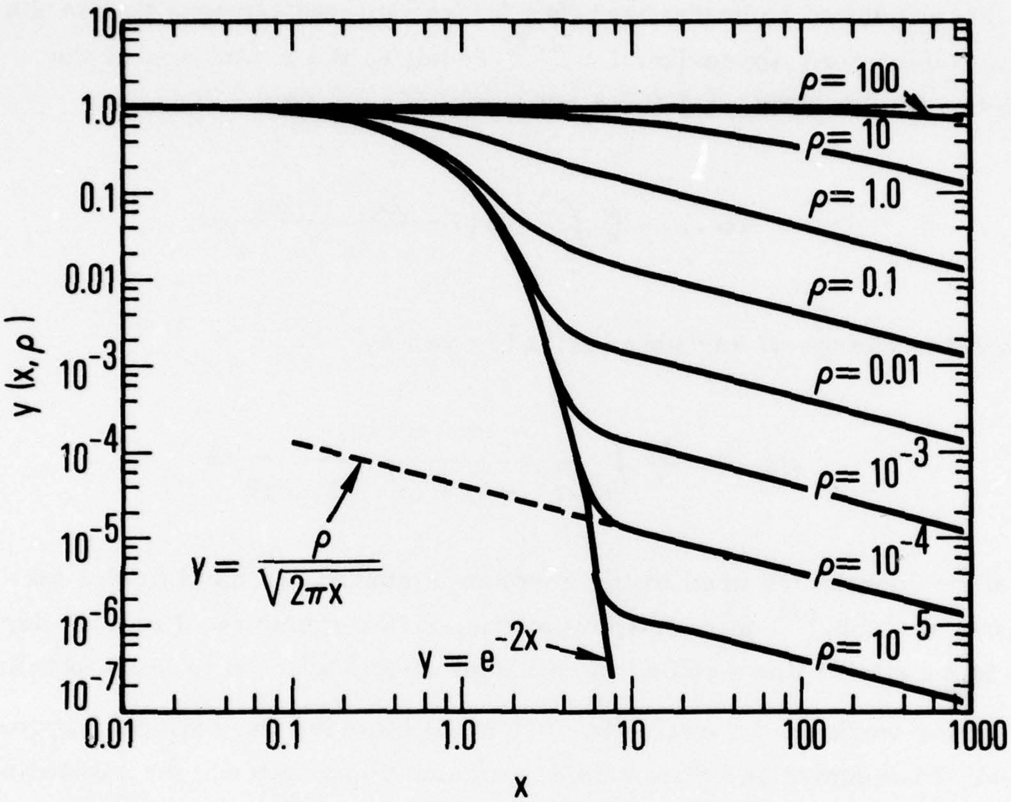

Fig. 1. The Function y(x, ρ). From Ref. 2.

$$
y(x,\rho) \rightarrow \begin{cases} 1 & x \rightarrow 0 \\ \rho/\sqrt{2\pi x} & x \rightarrow \infty \\ e^{-2x} & \rho \rightarrow 0 \\ e^{-x} I_0(x) & \rho \rightarrow 1 \\ 1 & \rho \rightarrow \infty \end{cases} \tag{2}
$$

where $I_0(x)$ is the modified Bessel function of order zero.

The dramatic difference in basic mathematical form that the function assumes in different regions of the $x\rho$ plane makes it impractical to use only one method of calculation. Six approximation expansions are used in the present method. These approximations are considered in the following section, and the regions in which they apply are indicated in Fig. 2.

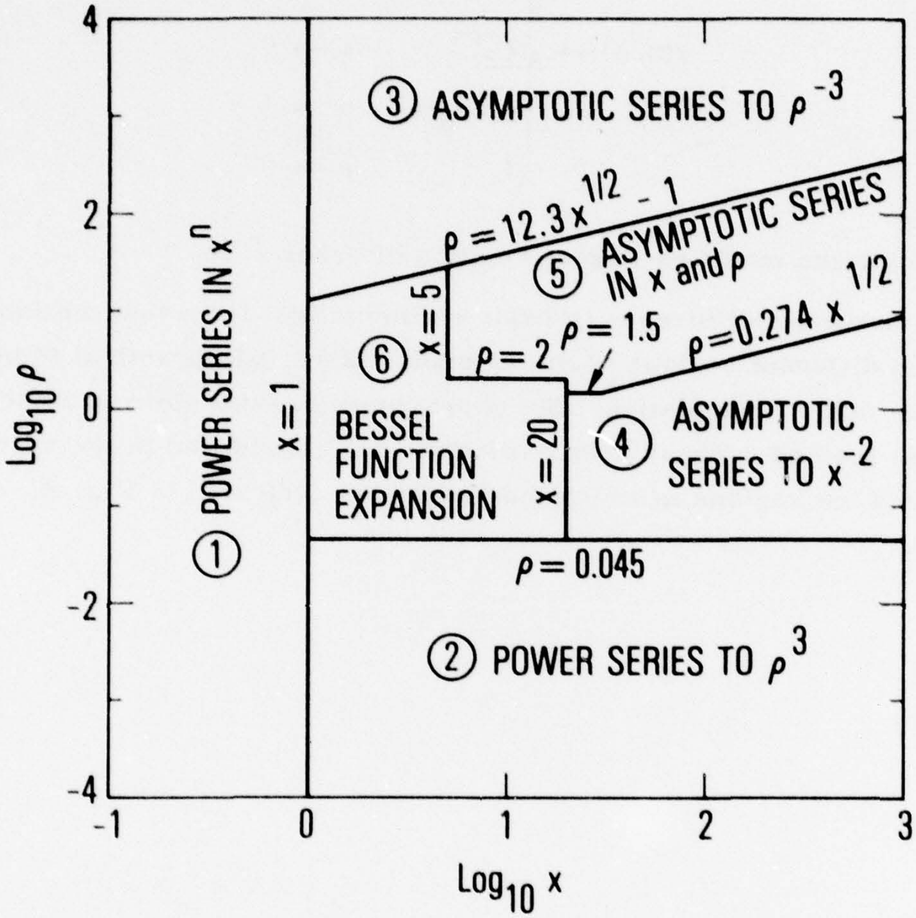

Fig. 2. Regions for which the Various Approximations to $y(x, \rho)$ Apply

METHODS OF COMPUTATION

A. EXPANSION FOR SMALL x (REGION 1)

For $x \le 1$, an expansion of the exponential factor of equation (1a) is made, and $y(x, \rho)$ is written as

$$y(x, \rho) = \sum_{n=0}^{\infty} (-1)^n \frac{(2x)^n}{n!} E_n(\rho) \tag{3}$$

where

$$E_n(\rho) = \frac{2}{\pi} \int_0^{\infty} \frac{dz}{(1 + z^2)(1 + \rho^2 z^2)^n}. \tag{4}$$

Explicit evaluation of $E_n(\rho)$ by the method of residues for the first few values of n leads by induction to the convenient recurrence relation

$$E_n(\rho) = \begin{cases} \dfrac{2n - 1}{2n} E_{n-1}(\rho) & \rho = 1 \quad (5a) \\[2ex] \dfrac{1}{\rho^2 - 1}\left[\rho C_n - E_{n-1}(\rho)\right] & \rho \neq 1 \quad (5b) \end{cases}$$

with

$$E_0(\rho) = 1 \text{ (for all } \rho),$$

$$C_n = \frac{2n - 3}{2n - 2} C_{n-1} = \frac{(2n - 3)!}{2^{2n-3}(n - 1)!(n - 2)!}, \tag{6}$$

and

$$C_1 = 1.$$

The explicit solutions for the first five $E_n(\rho)$ functions are

$$
\begin{aligned}
E_0(\rho) &= 1, \\
E_1(\rho) &= 1/(\rho + 1), \\
E_2(\rho) &= (\rho + 2)/2(\rho + 1)^2, \\
E_3(\rho) &= (3\rho^2 + 9\rho + 8)/8(1 + \rho)^3, \\
E_4(\rho) &= (5\rho^3 + 20\rho^2 + 29\rho + 16)/16(1 + \rho)^4.
\end{aligned}
\tag{7}
$$

Additional properties of $E_n(\rho)$ that can be derived are

$$
E_n(\rho) \rightarrow \begin{cases} 1 & \rho \rightarrow 0 \\ C_n/\rho & \rho \rightarrow \infty \\ C_{n+1} & \rho \rightarrow 1 \\ 1/\rho\sqrt{\pi n} & \rho \rightarrow \infty \end{cases}
\tag{8}
$$

In practice, $y(x, \rho)$ is computed from equation (3) and the recurrence relations equations (5) and (6). Since equation (3) is an alternating series of decreasing terms, the accuracy of the approximation can be checked as each term is added to the series by testing the absolute value of the term added. The slowest convergence of equation (3) occurs for $\rho = 0$, in which case terms through $n = 11$ must be retained for a relative accuracy of 0.01%. The forward recurrence relation equation (5b) is unstable for ρ near unity. For $|1 - \rho| \leq 0.044$, this stability sets in below $n = 11$. However, for this

condition of ρ and for $x \leq 1$, $y(x, \rho)$ may be computed to the desired accuracy with only the first two terms (i.e., $n = 0$ and 1) of the Bessel function expansion considered in the following section.

B. EXPANSION FOR SMALL ρ (REGION 2)

For this and the following three approximations, the starting point is Cobb's expansion[3] of $y(x, \rho)$ as a series of modified Bessel functions. The expansion is

$$y(x, \rho) = e^{-x}\left[I_0(x) + 2\sum_{n=1}^{\infty} \alpha^n I_n(x)\right] \tag{9}$$

where $\alpha = (\rho - 1)/(\rho + 1)$. For small ρ, $\alpha \to -1$, and we expand $y(x, \rho)$ in a Taylor series about $\alpha = -1$. At $\alpha = -1$, the series converges[4] to give $y(x, 0) = e^{-2x}$. The first derivative of equation (9) evaluated at $\alpha = -1$ is

$$\left.\frac{dy}{d\alpha}\right|_{\alpha = -1} = -2e^{-x}\sum_{n=1}^{\infty} n(-1)^n I_n(x). \tag{10}$$

Use of the recurrence relation[4]

$$I_n(x) = \frac{x}{2n}[I_{n-1}(x) - I_{n+1}(x)] \tag{11}$$

in equation (10) and shifts of summation indices such that the sums over I_{n-1} and I_{n+1} are transformed into sums over I_n yield

$$\left.\frac{dy}{d\alpha}\right|_{\alpha = -1} = xe^{-x}\left[\sum_{n=0}^{\infty} - \sum_{n=2}^{\infty}\right](-1)^n I_n(x) = xe^{-x}[I_0(x) - I_1(x)]. \tag{12}$$

Higher-order derivatives can be obtained by the same procedure. The resulting expansion to third order in ρ for y(x, ρ) is

$$y(x, \rho) = e^{-2x} + \left(\frac{2\rho}{1+\rho}\right) A_1 + \left(\frac{2\rho}{1+\rho}\right)^2 A_2 + \left(\frac{2\rho}{1+\rho}\right)^3 A_3 \qquad (13)$$

where

$$A_1 = xe^{-x}[I_0(x) - I_1(x)],$$

$$A_2 = \frac{A_1}{2} - \frac{x}{2}e^{-2x},$$

and

$$A_3 = -\frac{x}{6}e^{-x}[(2x - 3)I_0(x) - (2x - 2)I_1(x)] - \frac{x}{2}e^{-2x}.$$

The slowest rate of convergence of equation (13) occurs for large x. In this case, the coefficients A_n approach

$$A_n \sim \frac{1}{2^n\sqrt{2\pi x}} \qquad (14)$$

and successive coefficients decrease by the factor two. For smaller x, the decrease is faster. Thus, a worst case estimate of the accuracy of equation (13) can be obtained by substituting equation (14) into (13) to obtain

$$y = e^{-2x} + \frac{1}{\sqrt{2\pi x}}[\alpha + \alpha^2 + \alpha^3 + \alpha^4 + \cdots],$$

where $\alpha = \rho/(1 + \rho)$. If we retain only terms through α^3 in the sum, the absolute error of truncation is

$$\epsilon = \alpha^4 + \alpha^5 + \cdots = \frac{\alpha^4}{1 - \alpha}.$$

The largest α that can be tolerated for a maximum relative error of 10^{-4} (in the sum) is given by

$$(\alpha + \alpha^2 + \alpha^3) \geq 10^4 \frac{\alpha^4}{1 - \alpha}$$

for which $\alpha \leq 0.047$ ($\rho \leq 0.045$) is the solution. Similar analyses show that the α^3 term may be neglected for $\rho \leq 0.01$, and the α^2 term neglected when $\rho \leq 0.0001$.

Computation of the I_0 and I_1 Bessel functions required to evaluate A_1, A_2, and A_3 of equation (13) are handled with rational approximations(4) that provide sufficient accuracy for $1 \leq x \lesssim 20$. Beyond $x \simeq 20$, these rational approximations are not accurate enough to yield the difference $I_0 - I_1$ to sufficient accuracy. For $x \gtrsim 20$, use is made of the asymptotic expansion

$$y = e^{-2x} + \frac{1}{\sqrt{2\pi x}}\left[1 + \frac{3}{8x} + \frac{45}{128x^2}\right]\frac{\alpha}{2}\left(1 + \frac{\alpha}{2} + 0.266\alpha^2\right). \tag{15}$$

Up to the α^2 term, this expansion is obtained from equation (13) and the asymptotic expansions(4) for I_0 and I_1. The coefficient 0.266 on the α^3 term was determined empirically so as to yield 0.01% accuracy for all $x \geq 20$ and $\rho \leq 0.05$.

C. EXPANSION FOR LARGE ρ (REGION 3)

The expansion for this case is obtained exactly as for the small ρ expansion, except that the Taylor expansion is made about $\alpha = 1$. The result to third order in ρ^{-1} is [3]

$$y(x, \rho) = 1 - \left(\frac{2}{1+\rho}\right)B_1 + \left(\frac{2}{1+\rho}\right)^2 B_2 - \left(\frac{2}{1+\rho}\right)^3 B_3 \tag{16}$$

where

$$B_1 = xe^{-x}[I_0(x) + I_1(x)],$$

$$B_2 = \frac{x}{2} - \frac{B_1}{2},$$

and

$$B_3 = \frac{x}{6}e^{-x}[(2x+3)I_0(x) + (2x+2)I_1(x)] - \frac{x}{2}.$$

As for the small ρ expansion, the worst case of convergence of equation (16) occurs for large x. In this case, the first four coefficients approach

$$B_1 \sim \frac{1}{\sqrt{\pi}}(2x)^{1/2},$$

$$B_2 = \frac{1}{4}(2x),$$

$$B_3 \sim \frac{1}{6\sqrt{\pi}}(2x)^{3/2},$$

and

$$B_4 = \frac{1}{32}(2x)^2.$$

Substitution of these coefficients into equation (16) yields

$$y \sim 1 - \frac{2\alpha^{1/2}}{\sqrt{\pi}} + \alpha - \frac{4}{3\sqrt{\pi}}\alpha^{3/2} + \frac{\alpha^2}{2} - \ldots$$

where $\alpha = 2x/(\rho + 1)^2$. Since the series alternates in sign, we can be assured that the maximum absolute error incurred by truncating equation (16) at the cubed term is less than or equal to $\alpha^2/2$. The condition for relative error less than 0.01% is

$$\frac{\alpha^2}{2} \le 10^4\left[1 - \frac{2\alpha^{1/2}}{\sqrt{\pi}} + \alpha - \frac{8\alpha^{3/2}}{\sqrt{\pi}}\right]$$

from which we obtain $\alpha \le 0.01328$ or

$$\rho \ge 12.3x^{1/2} - 1.$$

In addition, the third; second; and first-order terms of equation (16) may be neglected, respectively, when

$$\rho \ge 28.2x^{1/2} - 1,$$

$$\rho \ge 142x^{1/2} - 1,$$

and

$$\rho \ge 16000x^{1/2} - 1.$$

As in the small ρ approximation, the functions I_0 and I_1 required to compute the B coefficients are obtained from accurate rational approximations.[4]

D. EXPANSION FOR LARGE x (REGION 4)

Substitution of the asymptotic expansions[4] for $I_n(x)$ into equation (9) and a collection of terms on like powers of x yields

$$y(x, \rho) \sim \frac{1}{\sqrt{2\pi x}}\left[\rho + \frac{F(\rho)}{8x} + \frac{G(\rho)}{2!(8x)^2} + \cdots\right] \tag{17}$$

where

$$F(\rho) = \left(\frac{\rho + 1}{2}\right)^3 [1 - 9\alpha - 9\alpha^2 + \alpha^3],$$

$$G(\rho) = \left(\frac{\rho + 1}{2}\right)^5 3[3 - 25\alpha + 150\alpha^2 + 150\alpha^3 - 25\alpha^4 + 3\alpha^5],$$

and $\alpha = (\rho - 1)/(\rho + 1)$. For $\rho \geqslant 1.225$, $F(\rho)$ is negative and decreases monatonically to $F = -2\rho^3$ as $\rho \to \infty$. Similarly, $G(\rho)$ is positive and increases monatonically to $G = 24\rho^5$ as $\rho \to \infty$. The next higher coefficient approaches $H = -720\rho^7$ for large ρ. Thus, the worst case of convergence for $\rho \geqslant 1.225$ appears to the alternating series

$$y \longrightarrow \frac{\rho}{\sqrt{2\pi x}}\left[1 - \frac{1}{2}\left(\frac{\rho^2}{2x}\right) + \frac{3}{4}\left(\frac{\rho^2}{2x}\right)^2 - \frac{15}{8}\left(\frac{\rho^2}{2x}\right)^3 + \cdots\right].$$

The absolute error of truncation at the x^{-2} term is less than $15(\rho^2/2x)^3/8$, and the condition for a relative accuracy of less than 0.01% is

$$\frac{15}{8}\left(\frac{\rho^2}{2x}\right)^3 \le 10^{-4}\left[1 - \frac{1}{2}\left(\frac{\rho^2}{2x}\right) + \frac{3}{4}\left(\frac{\rho^2}{2x}\right)^2\right],$$

which yields the condition $\rho^2/2x \le 0.0375$ or

$$x \ge 13.3\rho^2. \tag{18}$$

Comparisons of the results of equation (17) with exact calculations[2] confirm this bound by predicting the less stringent bound $x \ge 7.25\rho^{2.22}$ for $20 \le x \le 10^4$. In addition, these comparisons show that x must be greater than ~20 in order to obtain the desired accuracy of 0.01%. This result is consistent with equation (18) and the lower bound $\rho = 1.225$ set on ρ for this analysis.

For $\rho < 1.225$, the preceding error analysis does not apply because the series is not an alternating series. Here, comparisons with exact calculations confirm that equation (17) is accurate to the desired accuracy for $x \geqslant 20$ and ρ down to at least the upper bound ($\rho = 0.045$) of Region 2.

E. EXPANSION FOR LARGE x AND ρ (REGION 5)

The large x expansion equation (17) is restricted by the condition $\rho \le 0.274x^{1/2}$, whereas the large ρ expansion equation (16) is restricted by $\rho \ge 12.3x^{1/2} - 1$. The following method provides a means of computation in this excluded region. In equation (1a), we make the transformation

$$u = \frac{1}{\sqrt{1 + \rho^2 z^2}}$$

to obtain

$$y(x, \rho) = \frac{2\rho}{\pi}\int_0^1 \frac{f(u)}{\sqrt{1 - u^2}}\, du \tag{19}$$

where

$$f(u) = \frac{e^{-2xu^2}}{1 + u^2(\rho^2 - 1)}.$$

When x is large and $\rho > 1$, f(u) peaks sharply at $u = 0$, and most of the contribution to equation (19) will come from this region. This phenomenon suggests that not much error will result if we set the upper limit of integration to infinity and expand the square root term of equation (19) in a power series. This latter expansion is

$$\frac{1}{\sqrt{1 - u^2}} = \sum_{n=0}^{\infty} B_n u^{2n}. \tag{20}$$

The expansion coefficient B_n is

$$B_n = \frac{(2n)!}{2^{2n}(n!)^2},$$

which, for computational purposes, can be written in the recurrence form

$$B_n = \left(\frac{2n - 1}{2n}\right) B_{n-1} \tag{21}$$

with

$$B_0 = 1.$$

Substitution of equation (20) into (19), an interchange of the orders of integration and summation, and setting the upper limit of integration to infinity yields

$$y(x, \rho) = \frac{2\rho}{\pi} \sum_{n=0}^{\infty} B_n \int_0^{\infty} \frac{u^{2n} e^{-2xu^2}}{1 + u^2(\rho^2 - 1)} du.$$

With the transformation $z = u\sqrt{\rho^2 - 1}$, this becomes

$$y(x, \rho) = \rho \sum_{n=0}^{\infty} \frac{B_n F_n(\alpha)}{(\rho^2 - 1)^{n+1/2}}, \tag{22}$$

where

$$F_n(\alpha) = \frac{2}{\pi} \int_0^{\infty} \frac{z^{2n} e^{-\alpha^2 z^2}}{1 + z^2} dz \tag{23}$$

and

$$\alpha = \sqrt{\frac{2x}{\rho^2 - 1}}.$$

A recurrence relation can be obtained for $F_n(\alpha)$ as follows. Differentiate equation (23) with respect to α to obtain

$$F_n(\alpha) = -\frac{1}{2\alpha} \frac{dF_{n-1}(\alpha)}{d\alpha}. \tag{24}$$

From the solution[5]

$$F_0(\alpha) = e^{\alpha^2}[1 - \mathrm{erf}(\alpha)], \tag{25}$$

equation (24) can be used to evaluate the first few $F_n(\alpha)$ functions, from which, by induction, we can obtain either the explicit solution

$$F_n(\alpha) = (-1)^n \left[F_0(\alpha) \times \frac{2}{\sqrt{\pi}} \sum_{i=1}^{n} (-1)^i \frac{(2i-1)(2i-3)\cdots 5 \cdot 3 \cdot 1}{2^i \alpha^{(2i-1)}(2i-1)} \right]$$

or the recurrence relations

$$F_n(\alpha) = C_n(\alpha) - F_{n-1}(\alpha) \tag{26}$$

and

$$C_n(\alpha) = \frac{2n-3}{2\alpha^2} C_{n-1}(\alpha)$$

with

$$C_1(\alpha) = \frac{1}{\sqrt{\pi}\alpha} .$$

In application, $y(x, \rho)$ is computed from equation (22) with B_n evaluated by equation (21) and $F_n(\alpha)$ by equations (25) and (26).

The accuracy of this expansion was determined by comparison with exact calculations. In the region $x \geq 5$ and $\rho \geq \sqrt{2}$, the approximation yields the desired accuracy with only a few terms in the expansion. Near $x = 5$, $\rho = \sqrt{2}$, about ten terms are required, whereas for $x \geq 10^4$ or $\rho \geq 2 \times 10^3$ (and $x \geq 1$), only the first term of equation (22) is required, i.e.,

$$y \sim e^{\alpha^2} [1 - \operatorname{erf}\alpha].$$

In practice, the sum is terminated when the relative term contribution to the accumulated sum is less than 10^{-6}.

Computation of the function $F_0(\alpha)$ defined by equation (25) is made to a relative accuracy of 5×10^{-6} by using the approximation of Matta and Reichel.[6]

F. INTERMEDIATE x AND ρ (REGION 6)

For intermediate values of x and ρ, none of the methods considered to now can yield the accuracy desired in $y(x, \rho)$. For this excluded region (Region 6), we resort to the Bessel function expansion equation (9)

$$y(x, \rho) = e^{-x}\left[I_0(x) + 2\sum_{n=1}^{N}\left(\frac{\rho - 1}{\rho + 1}\right)^n I_n(x)\right]. \qquad (27)$$

Although this expression (with $N \to \infty$) is an exact solution of equation (1), its use for efficient computation is limited, especially for large x, unless ρ is very close to unity. For large x, the functions $I_n(x)$ fall off very slowly with n, and, consequently, a very large number of terms must be included in the summation. The number of terms (N) that must be included within Region 6 for a relative accuracy of 0.01% are tabulated in Table 1. Even for x only as large as 20, as many as 27 terms must be included for the desired accuracy.

In practice, the number of terms used in the expansion is determined by the worst case of $\rho \sim 0.05$, for which

$$N \simeq 8x^{0.393}.$$

The Bessel functions $I_n(x)$ are computed with a backward recurrence algorithm[7] initiated at order

$$M = 14x^{0.307}$$

to ensure 10^{-4} relative accuracy in $I_n(x)$ through $n = N$.

Table 1. Number of terms required in Bessel function expansion of $y(x, \rho)$ for 0.01% accuracy.

ρ	x = 1	2	5	10	20
20		9	13		
10	7	9	12		
5	7	8	11		
2	6	7	8	10	11
1	1	1	1	1	1
0.5	6	7	9	10	11
0.2	7	9	12	15	19
0.1	8	10	14	18	23
0.05	8	10	15	19	26

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Electronics Research Laboratory: Electromagnetic theory, devices, and propagation phenomena, including plasma electromagnetics; quantum electronics, lasers, and electro-optics; communication sciences, applied electronics, semiconducting, superconducting, and crystal device physics, optical and acoustical imaging; atmospheric pollution; millimeter wave and far-infrared technology.

Materials Sciences Laboratory: Development of new materials; metal matrix composites and new forms of carbon; test and evaluation of graphite and ceramics in reentry; spacecraft materials and electronic components in nuclear weapons environment; application of fracture mechanics to stress corrosion and fatigue-induced fractures in structural metals.

Space Sciences Laboratory: Atmospheric and ionospheric physics, radiation from the atmosphere, density and composition of the atmosphere, aurorae and airglow; magnetospheric physics, cosmic rays, generation and propagation of plasma waves in the magnetosphere; solar physics, studies of solar magnetic fields; space astronomy, x-ray astronomy; the effects of nuclear explosions, magnetic storms, and solar activity on the earth's atmosphere, ionosphere, and magnetosphere; the effects of optical, electromagnetic, and particulate radiations in space on space systems.

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